Applying Dispersive Changes to Lagrangian Particles in Groundwater Transport Models

Leonard F. Konikow

Abstract   Method-of-characteristics groundwater transport models require that changes in concentrations computed within an Eulerian framework to account for dispersion be transferred to moving particles used to simulate advective transport. A new algorithm was developed to accomplish this transfer between nodal values and advecting particles more precisely and realistically compared to currently used methods. The new method scales the changes and adjustments of particle concentrations relative to limiting bounds of concentration values determined from the population of adjacent nodal values. The method precludes unrealistic undershoot or overshoot for concentrations of individual particles. In the new method, if dispersion causes cell concentrations to decrease during a time step, those particles in the cell having the highest concentration will decrease the most, and those with the lowest concentration will decrease the least. The converse is true if dispersion is causing concentrations to increase. Furthermore, if the initial concentration on a particle is outside the range of the adjacent nodal values, it will automatically be adjusted in the direction of the acceptable range of values. The new method is inherently mass conservative.

1 Introduction

The groundwater solute-transport equation can be difficult to solve numerically—especially relative to the state of the art in numerically solving the governing groundwater flow equation—because its mathematical character can vary from parabolic to hyperbolic depending on the relative strength of advection to dispersion (e.g., Konikow et al. 2007). Consequently, a suite of alternative numerical methods have evolved for developing and applying simulation models to subsurface contaminant transport problems. One broad class includes mixed Eulerian–Lagrangian methods, generally in which the advective and dispersive terms of

L. F. Konikow (✉)
U.S. Geological Survey, 431 National Center, Reston, VA 20192, USA
e-mail: lkonikow@usgs.gov

the governing solute-transport equation are split and solved separately. But a problematic issue with operator splitting is the reconnection of the separated effects into a total solution. A popular subset of this class of mixed methods includes the method-of-characteristics (MOC) approach and related particle methods, which have been widely used for decades (e.g., Garder et al. 1964; Pinder and Cooper 1970; Bredehoeft and Pinder 1973; Konikow and Bredehoeft 1978; Zheng 1990; Konikow et al. 1996; Zheng and Wang 1999; Oude Essink 2001; Zimmermann et al. 2001).

MOC models have the ability to accurately track the migration of sharp fronts through a flow system with a minimum of numerical dispersion. MOC models generally use particle tracking to represent advective transport and finite-difference methods to simulate concentration changes arising from dispersion and mixing processes. However, for the method to work well, there has to be a reliable and accurate transfer of information between the split operators. That is, if concentration changes due to dispersion are computed for cells or nodes of a finite-difference grid, those changes have to be applied to the particles used to track the advective movement of solute, and vice versa.

Zheng and Bennett (1995) describe a relatively simple approach in which the change in concentration computed for a cell is applied to all moving particles located within that cell at a particular time. If the calculated change in concentration during a time increment is positive (i.e., increasing), that change is added to the concentration of all particles in the cell. This conserves mass, though if there is a range in concentration values associated with the various particles, the uniform addition of a constant value may lead to a small amount of numerical dispersion because there is no spatial gradient preserved for the concentration change. If the change in concentration in a cell is negative, however, that decrease is applied to particles in the cell on a percentage basis. This approach is better than straight subtraction of the decrease because it precludes positive particle concentrations from going negative. This percentage (or weighted) reduction in concentration will result in a greater absolute concentration decrease on particles having higher concentration values and smaller absolute reductions on particles having lower values within the cell, which are conditions expected in a cell in which there is a net dispersive flux of solute out of the cell. This approach also preserves a mass balance within a cell. Zheng and Bennett (2002) also note that for negative changes in concentration, another approach is to remove all particles in the cell and replace them with a new set of particles that are all assigned the concentration of the cell. The downside of this is that it eliminates all concentration gradients within the cell that otherwise would be preserved on the particles, thereby locally minimizing or eliminating the benefits of advective particle tracking.

An alternative approach is to compute the change in concentration due to dispersion directly at the location of the particles. Zimmermann et al. (2001) describe the implementation of the particle strength exchange method, which offers more precision and accuracy overall, but would be computationally intensive for a three-dimensional problem. In fact, the implementation of Zimmermann et al. (2001) was solely for a 2D model.

The purpose of this article is to describe and document a new and improved method in numerical transport modeling to transfer concentration changes (due to dispersion and other processes) calculated for grid cells to the concentrations on particles used to represent advective transport. The new method incorporates improvements for cases of both increasing and decreasing cell values due to dispersion or other terms and is straightforward to implement in a 3D transport model.

2 Solute-Transport Equation

The theoretical basis for the equation describing solute transport has been well documented in the literature (e.g., Bear 1972, 1979; Domenico and Schwartz 1998). A commonly accepted generalized form of the transport equation for a single solute species subject to decay and linear, reversible, equilibrium sorption effects may be expressed as:

$$\frac{\partial(\varepsilon C)}{\partial t} = \frac{1}{R_f}\frac{\partial}{\partial x_i}\left(\varepsilon D_{ij}\frac{\partial C}{\partial x_j}\right) - \frac{1}{R_f}\frac{\partial}{\partial x_i}\left(\varepsilon C V_i\right) - \frac{C'W^*}{R_f} - \lambda\varepsilon C \tag{1}$$

where C is the volumetric concentration (mass of solute per unit volume of fluid, ML^{-3}); ε is the effective porosity of the porous medium (dimensionless); D_{ij} is the coefficient of hydrodynamic dispersion (a second-order tensor), L^2T^{-1}; V_i is the seepage velocity (or average interstitial velocity), LT^{-1}; t is time, T; W^* is the volumetric flux per unit volume (positive for outflow and negative for inflow), T^{-1}; λ is the decay rate, T^{-1}; R_f is the retardation factor (dimensionless); and C' is the concentration of the solute in the source or sink fluid, ML^{-3}.

3 Numerical Methods

The method-of-characteristics tracks a set of moving particles through a fixed spatial grid (see Konikow et al. 1996). Each particle has a location and concentration (or mass) associated with it. Konikow et al. (1996) show that the change in concentration of a reference point moving with the retarded velocity of groundwater can be represented by the material derivative as:

$$\frac{dC}{dt} = \frac{1}{\varepsilon R_f}\frac{\partial}{\partial x_i}\left(\varepsilon D_{ij}\frac{\partial C}{\partial x_j}\right) + \frac{\sum\left[W(C'-C)\right]}{\varepsilon R_f} - \lambda C \tag{2}$$

The change in concentration due to dispersion, sources, and decay within the area of a finite-difference cell can be calculated by solving Eq. 2 using explicit or implicit finite-difference methods, assuming that the concentrations are the averages of concentrations of all particles located within a cell. The concentration changes must then be applied to all particles located within the cell before the next advective time step is taken.

4 Applying Dispersive Flux to Particles

In applying concentration changes to particles within a cell, an overriding consideration is that this transfer must conserve mass, and, hence, the sum of the changes in mass on the particles must equal the change in mass computed for the cell. Another objective is to preserve concentration gradients within a cell as reflected in concentration differences among particles. One concern is that because the particle concentrations will usually include a range of concentration values about the mean of the cell, the adjustment of particle concentrations for the change due to dispersion might cause the concentration of individual particles to decrease to a negative value or to increase to a value higher than the highest source concentration. Such unrealistic undershoot and overshoot would propagate spatially and temporally as particles move with the flow.

Recognizing that individual particle concentrations can deviate from the mean concentration of the cell, and that according to the governing equation the dispersive flux is driven by
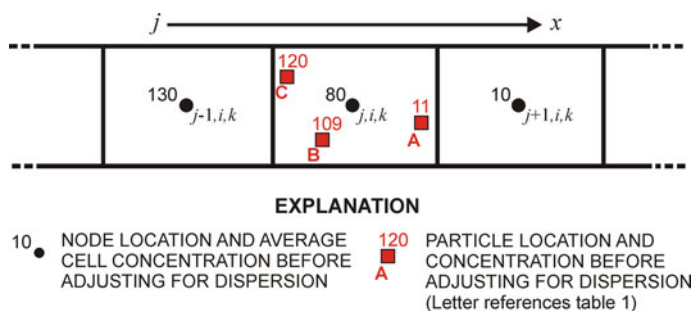
Fig. 1 Part of one-dimensional grid illustrating simple example for a cell containing three particles and subject to a decrease in cell concentration due to dispersion during the time increment

the concentration gradient, we can deduce that the appropriate change in concentration on a particle should be related to both the magnitude of its concentration and the mean concentration in the cell. That is, if the computed change in concentration due to dispersion in a cell is negative (cell concentration decreases), then particles within that cell that have high concentrations relative to the mean should show a greater reduction in concentration than particles having a relatively low concentration. This is expected because the concentration difference (and gradient) driving the dispersive flux would be greatest for a particle having the highest concentration. Conversely, if the computed change in concentration due to dispersion in a cell is positive (an increase in concentration), then particles within that cell that have a relatively low concentration should show a greater increase in concentration than particles having a relatively high concentration. In this case, this occurs because the concentration difference driving the dispersive flux would be greatest for a particle having the lowest concentration.

4.1 Decreasing Concentration

If dispersion indicates that the concentration of a cell should decrease over a time increment because the dispersive flux out of the cell is greater than the dispersive flux into the cell, and the cell contains a number of particles of varying individual concentrations, then a simple approach is to subtract the same change in concentration calculated for the cell from the concentration of each particle. This would assure that the mean of the changed concentrations of all the particles ($\bar{C}_P$) would equal the new cell concentration (C_{jik}^{n+1}) and that the process would necessarily conserve mass. (Note that the *jik* notation reflects the column-row-layer labeling convention of MODFLOW (McDonald and Harbaugh 1988), which uses a block-centered finite-difference grid.)

A simple hypothetical example illustrating a part of a simple one-dimensional grid is shown in Fig. 1. In this example, cell *j, i, k* has a mean concentration of 80 and includes three particles, which have concentrations of 11, 109, and 120. The concentration gradient toward the forward cell is greater in magnitude than that with the backward cell, so that difference will govern the net change in concentration at the cell due to dispersion, and this example would represent a net decrease in concentration at cell *j, i, k*. If the net change at the cell were equal to −12 and it was applied equally to each particle in the cell, it would result in the concentration of one of the particles becoming negative in value (see Table 1, column 2). Of course, the mean concentration of the three particles (68.0) would still equal the new concentration for the cell at the end of the time increment (C_{jik}^{n+1}).

Table 1 Results of three different methods for computing change in concentration on particles due to dispersion from time level n to time level $n + 1$ for cell j, i, k in problem shown in Fig. 1, where $\Delta C = -12$

	C^n	C^{n+1}		
		$C^n + \Delta C$	$C^n + C^n \times (\%\Delta C)^a$	$C^n + (\text{scaled } \%\Delta C)^b$
CELL	80	68	68	68
Pt. A	11	−1	9.35	10.83
Pt. B	109	97	92.65	92.03
Pt. C	120	108	102	101.14
$\bar{C}_P$	80	68	68	68

[a] $(\%\Delta C) = (\Delta C/C_{jik}^n) = -0.15$

[b] Calculated using Eq. 3

In both the original MOC3D code (Konikow et al. 1996) and its predecessor two-dimensional MOC code (Konikow and Bredehoeft 1978), the method for applying the change in concentration for the cell to particles in the cell if the concentration was decreasing was to reduce the concentrations of all particles in the cell by the percentage reduction calculated for the cell (% ΔC). Reducing the concentration at particles by the percentage of the reduction at the cell is equivalent to using the value of zero as a base or limit to the amount of decrease that can occur on a particle. This had the advantage that as long as particles have a concentration greater than zero, the change could not cause the new concentration to become negative. In the simple example represented by Fig. 1 and Table 1, this approach would indicate a reduction of 15% of the cell concentration [column 4: $C^n - (\%\Delta C)$], resulting in a final concentration of 68, the same as before. Applying the same percentage reduction to all of the particles in the cell, however, results in a greater absolute decrease in the particles having a higher concentration and avoids the particle with the lowest concentration (Particle A) being reduced to a value below zero (Table 1, column 3: $C^n - \Delta C$).

Note that by reducing the concentration of Particle A by a percentage, its new concentration (9.35) remains less than the concentration of the forward cell (10.0), which was the lower limit of the concentration difference driving the dispersive decrease in concentration in cell j, i, k. Thus, it can be argued that when dispersion induces a decrease in concentration in a cell, the base should actually be the minimum concentration occurring in any adjacent (neighboring) cell. In the example shown in Fig. 1, the base would be the concentration in the forward cell ($C = 10$). Accordingly, the percentage reduction can be scaled to this minimum concentration as a base and would be directly related to the ratio $\Delta C/\left(C_{jik}^n - C_{\min}\right)$, where $C_{\min}$ is the minimum nodal concentration in any cell adjacent to cell j, i, k that is used in the calculation of dispersive flux. For a three-dimensional finite-difference grid, accounting for cross-product terms, this could include as many as 26 adjacent cells.

The concentration at any particle or any node can thereby be computed directly from:

$$C_P^{n+1} = \left(C_P^n - C_{\min}\right)\left(1 + \left[\Delta C/(C_{jik}^n - C_{\min})\right]\right) + C_{\min}. \tag{3}$$

The results of applying Eq. 3 to the example problem are shown in column 5 of Table 1 (scaled % ΔC) and lead to the greatest reduction in the concentration of the particle with the highest initial concentration, as well as the smallest reduction in the concentration of the particle with the lowest initial concentration. This smaller range in concentration change serves to minimize any possible numerical dispersion arising from the transfer of dispersive

changes from nodes to particles. Furthermore, the final concentration of the particle with the lowest concentration remains greater than the minimum concentration of the adjacent cells, which is a desired end result of using this new algorithm.

In the event that a particle had a concentration less than the base level (C_{min}) at the beginning of the time increment, this mass-conservative algorithm has the advantage that it will compute an increase in concentration for such a particle even though the cell concentration is decreasing. This self-correcting aspect minimizes the potential for the propagation of oscillations. For example, for the problem illustrated in Fig. 1 and Table 1, assume that a particle in the cell had a concentration at the start of the time increment (n) of either 5 or -5. Then its concentration at the end of the time increment ($n+1$) computed using a straight percentage reduction would have been 4.25 and -4.25, respectively. On the other hand, computing the change using Eq. 3 would result in a concentration at the end of the time increment of 6.57 and -2.43, respectively. In both cases, the final concentration would have been closer to the base value of 10 when Eq. 3 is used compared to the two alternative approaches.

The use of Eq. 3 produces results that are more consistent with conceptual expectations for the dispersion process when concentrations are decreasing due to dispersion and cannot create particle concentrations that undershoot physically based bounds on the basis of the transfer. Hence, the new algorithm is preferable to the alternatives considered.

4.2 Increasing Concentration

If dispersion indicates that the concentration of a cell should increase over a time increment because the dispersive flux out of the cell is less than the dispersive flux into the cell, then the new concentration for the cell at the end of the time increment, represented by the nodal value, would be $C_{jik}^{n+1} = C_{jik}^{n} + \Delta C_{jik}$. At the start of the calculation of dispersive fluxes for the time increment, the cell contains a number of particles of varying individual concentrations, whose mean equals C_{jik}^{n}. To apply the calculated change in concentration in the cell to the particles in that cell, the simplest approach would be to add the same change in concentration calculated for the cell to the concentration of each particle. This would assure that the mean of the new concentrations of all the particles ($\bar{C}_P$) would equal the new cell concentration (C_{jik}^{n+1}) and that the process would necessarily conserve mass. This was the method used in both the original MOC3D code (Konikow et al. 1996) and its predecessor two-dimensional MOC code (Konikow and Bredehoeft 1978). However, this computationally simple approach can lead to individual particle concentrations that are higher than the value of the highest concentration used to compute the dispersive flux from an adjacent cell into cell j, i, k. But just as C_{min} represents a lower limit to updated particle concentrations when cell concentrations are decreasing due to dispersion, as described in the preceding section, so should the highest concentration in an adjacent cell represent an upper limit to increased particle concentrations.

Thus, a new method was developed for increasing individual particle concentrations in a cell where dispersion is causing a net flux of mass into the cell. Analogous to the method used when concentrations are decreasing, the new method increases concentrations on particles on a percentage basis over a scaled range where the maximum concentration in any adjacent cell (C_{max}) represents the theoretical upper limit for increased particle concentrations. This method has the following characteristics and constraints:

(1) Particles with a concentration greater than the mean concentration at the cell node (C_{jik}^{n}) should increase less than the nodal increase, with the particle having the highest concentration increasing the least.

(2) Particles with a concentration less than the mean concentration at the cell node should increase more than the nodal increase, with the particle having the lowest concentration increasing the most.

(3) Particles with a concentration equal to C_{max} should not change in value, even though the mean cell concentration is increasing.

(4) Particles with a concentration equal to C_{jik}^n should increase by the same amount as at the node (ΔC_{jik}).

(5) Particles with a concentration already above C_{max} should decrease in concentration.

(6) The mean of the particle concentrations at the end of the time increment should equal the new concentration at the node (C_{jik}^{n+1}) (that is, the application of the dispersive change to particles should be mass conservative).

We can meet these objectives (or constraints) by developing an algorithm that first increases the particle concentration by some constant amount (C_x) more than the computed nodal increase (ΔC) and then subsequently reducing the temporarily overestimated particle concentration on a percentage basis, where the fractional reduction is related to the ratio of C_x to $\left(C_{jik}^n + \Delta C + C_x \right)$.

The fourth condition listed above can thereby be expressed mathematically as:

$$\left(C_{jik}^n + \Delta C + C_x \right) \left(1 - \frac{C_x}{C_{jik}^n + \Delta C + C_x} \right) = C_{jik}^n + \Delta C \tag{4}$$

Next, we must determine the value of C_x. Based on the third constraint above, we can express Eq. 4 for a particle having a value of C_{max}. For this case, Eq. 4 can be rewritten as:

$$(C_{max} + \Delta C + C_x) \left(1 - \frac{C_x}{C_{jik}^n + \Delta C + C_x} \right) = C_{max} \tag{5}$$

Solving Eq. 5 for the unknown quantity, C_x, results in:

$$C_x = \frac{-C_{jik}^n \Delta C - (\Delta C)^2}{C_{jik}^n + \Delta C - C_{max}} \tag{6}$$

Once C_x is defined for a particular cell and time increment on the basis of the local C_{max}, then the new concentration for any given particle in the cell can be calculated from the following generalized version of Eq. 4:

$$C_{PT}^{n+1} = \left(C_{PT}^n + \Delta C + C_x \right) \left(1 - \frac{C_x}{C_{jik}^n + \Delta C + C_x} \right) \tag{7}$$

As an example, consider a simple hypothetical problem illustrating a part of a two-dimensional grid in which the cell to cell concentration gradients indicate that the concentration for a cell of interest (j, i, k) should increase during the time increment (see Fig. 2). In this example, the cell has a mean concentration of 100 and $\Delta C = +20$. Figure 3 shows that this cell includes eight particles, which have concentrations ranging from 10 to 500 and a mean of 100. If the net change at the cell was applied equally to each particle in the cell, as is commonly done, it would result in the concentration at the end of the time increment of one of the particles (Pt. A) becoming higher than that of the adjacent cell with the highest concentration (see Table 2, column 3: $C^n + \Delta C$). Because the latter is driving the dispersive increase in concentration, it is physically unreasonable for any particle to increase to a level greater than that driving the change.
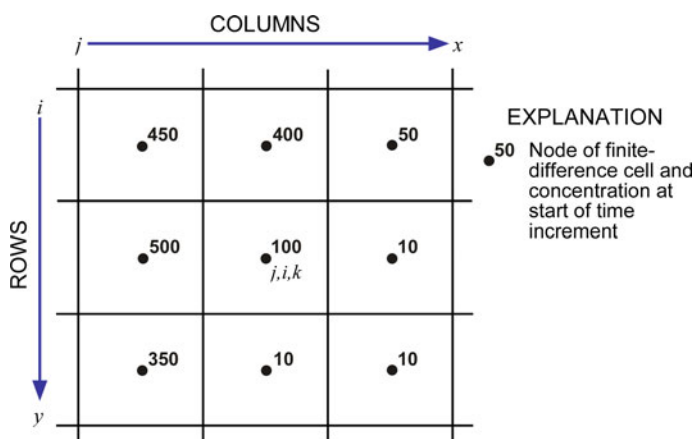
Fig. 2 Part of a two-dimensional grid illustrating concentration gradients between cell *j, i, k* and the eight adjacent cells for a case in which the cell concentration will increase during a time increment because of dispersion
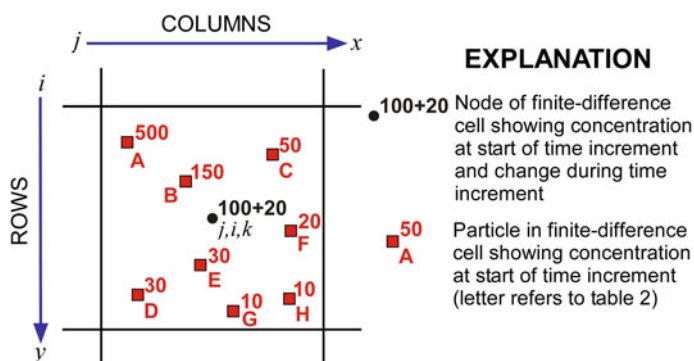

Fig. 3 Closer view of cell *j, i, k* from Fig. 2 showing hypothetical distribution of particles in the cell and their individual concentrations, which have a mean concentration of 100 at the start of the time increment. In this example, the cell concentration increases by 20 during the time increment because of the net dispersive flux from adjacent cells

As an alternative, we can compute the new concentrations of the individual particles by a percentage over the scaled range using Eqs. 6 and 7. In this case, application of Eq. 6 would indicate a value of $C_x \cong 6.316$. The results of then applying Eq. 7 are shown in column 4 of Table 2 (C^n + scaled%ΔC). They show the desirable characteristics that (1) the greatest absolute increase occurs on the particles with the lowest concentration at the beginning of the time increment, (2) smaller actual increases occur on particles with higher concentrations, and (3) the particle having a concentration equal to that of the highest concentration in an adjacent cell shows no increase in concentration. Of course, the mean of the concentrations of the eight particles at the end of the time increment ($\bar{C}_P$) must and does equal the new nodal concentration (C_{jik}^{n+1}), indicating that the application of the new method is mass conservative.

If this cell had included a particle with $C^n = 0$, its concentration would have increased to $C^{n+1} = 25$. If this cell had included a particle with a negative concentration, say $C^n = -10$, its concentration would have increased to $C^{n+1} = 15.5$. If this cell had included a particle

Table 2 Results of two different methods for computing change in concentration on particles due to dispersion from time level n to time level $n+1$ for cell j, i, k for two-dimensional example problem illustrated in Figs. 2 and 3, where $\Delta C = +20$

| | C^n | C^{n+1} | |
		$C^n + \Delta C$	$C^n + (\text{scaled } \%\Delta C)$ [a]
CELL	100	120	120.0
Pt. A	500	520	500.0
Pt. B	150	170	167.5
Pt. C	50	70	72.5
Pt. D	30	50	53.5
Pt. E	30	50	53.5
Pt. F	20	40	44.0
Pt. G	10	30	34.5
Pt. H	10	30	34.5
$\bar{C}_P$	100	120	120.0

[a] Calculated using Eqs. 6 and 7

with a concentration already greater than that in the highest adjacent cell, say $C^n = 600$, then its concentration would be computed to slightly decrease to $C^{n+1} = 595$, even though the cell concentration is increasing.

As was true for Eq. 3, the use of Eqs. 6 and 7 also produces results that are more consistent with conceptual expectations for the dispersion process and the transfer process cannot create particle concentrations that overshoot physically based bounds. Hence, it is preferable.

5 Example Problems

Examples based on a benchmark problem described by Konikow et al. (1996) are used to illustrate some aspects of the new method (although a variety of test cases would be required to illustrate a comprehensive range of issues). The selected problem includes three-dimensional solute transport of a nonreactive constituent from an instantaneous point source, or Dirac initial condition, in a uniform steady flow field in a homogeneous porous medium. An analytical solution is provided by Wexler (1992), and its application is described by Konikow et al. (1996). The explicit MOC method of Konikow et al. (1996) was modified to incorporate the new method of adjusting particle concentrations, and the results compared to the original method.

The properties of the test case are summarized in Table 3 and described in more detail by Konikow et al. (1996); however, this application differs from Konikow et al. (1996) in that the dispersivity values were increased (from $\alpha_L = 1.0$ m and $\alpha_T = 0.1$ m) and the simulation time was increased to 120 days (from 90 days). The numerical solution was generated on a $72 \times 72 \times 25$ grid with a grid spacing of 3.333 m in the horizontal (x- and y-) directions and 10 m in the vertical direction using 15 particles per cell and a Courant criterion of 0.25. The numerical solution compares very closely to the analytical solution, although the numerical solution exhibits slightly greater spreading, particularly in the trailing part of the plume (Fig. 4). However, after 120 days, the differences between the two numerical solutions (using the old and the new particle adjustment algorithms) were too small to discern on the contour

Table 3 Properties of test problem for 3D transport from an initial point source

Parameter	Value
Hydraulic conductivity (K)	1.0 m/d
Porosity (ε)	0.1
Longitudinal dispersivity (α_L)	2.0 m
Transverse dispersivity (α_T)	0.4 m
Velocity (V_x)	1.0 m/d
Initial mass	1×10^7
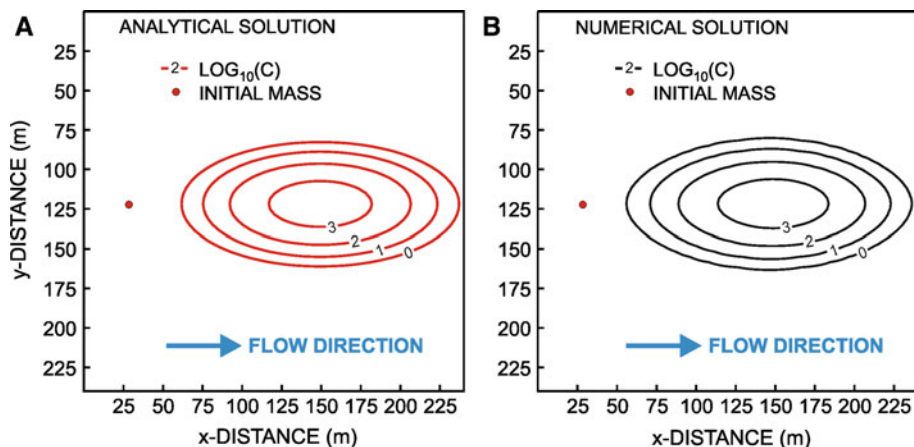
Fig. 4 Comparison of analytical (**a**) and numerical (**b**) solutions for a test problem with three-dimensional solute transport of an initial point source in a uniform flow field for 120 days

plot. Nevertheless, there were measureable differences in particle concentrations between the two (Fig. 5). The differences between the original and new algorithms were characterized by computing the change in concentration to be applied to each particle at a given time step using both the old and new methods, but in a simulation in which concentrations are advanced in time using the new method; note therefore that the differences shown in Fig. 5 do not represent cumulative changes, but only discrete differences for each point in time. The mean differences are shown separately for particles that decreased in concentration and those that increased in concentration. The average difference for a particular time step exceeds one percent during early time steps, but the average difference tends to decrease with time as the plume disperses and concentration gradients decrease. It was anticipated that the effect would be larger for heterogeneous media, and this was confirmed by modifying the test case to incorporate about 10 small clusters of cells with hydraulic conductivities that were up to a factor of 5 different than that for the homogeneous case.

With some heterogeneity introduced into the system, the resulting 3D flow field is no longer uniform. After 120 days of simulated time has elapsed, small differences in the numerical solutions are visible in the contoured concentration distributions (Fig. 6), even using the original slightly smaller dispersivity values ($\alpha_L = 1.0$ m and $\alpha_T = 0.1$ m). This further indicates that the new algorithm is more important when simulating solute transport in more realistic, complex, heterogeneous, transient field problems than in simple idealized systems.
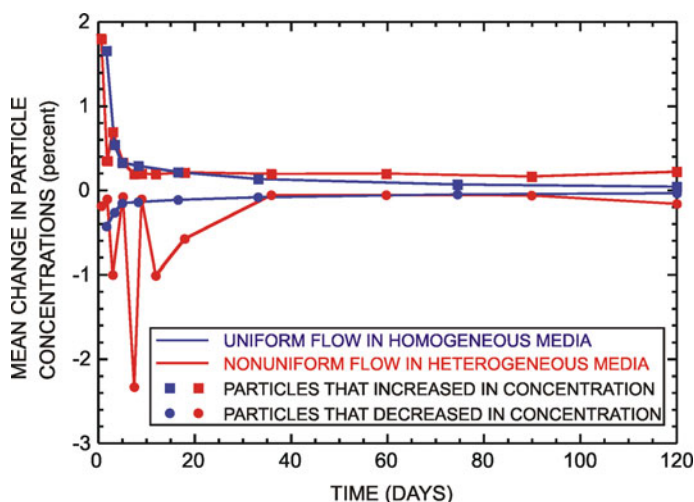
Fig. 5 Comparison of effect of new algorithm on particle concentrations during particular time steps during the numerical solution using the method of characteristics for both homogeneous and heterogeneous variants of the test case
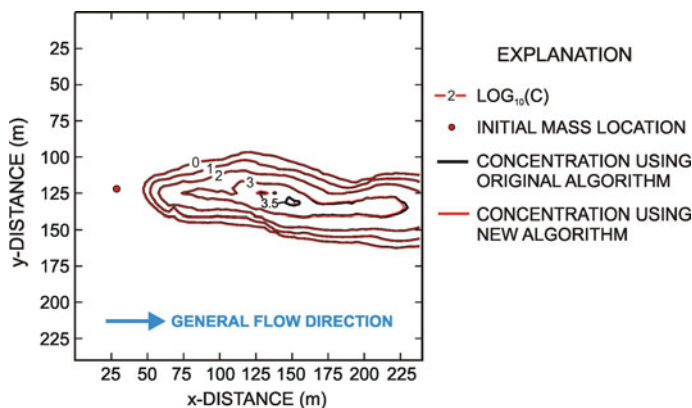

Fig. 6 Comparison of calculated plumes after 120 days computed using both original and new algorithms for adjusting particle concentrations in MOC numerical solutions for case with added heterogeneity in porous media for a test problem with three-dimensional solute transport of an initial point source

The test case illustrated in Fig. 5 was also modified so that flow was at a 45-degree angle to the grid and $V_x = V_y = 1.0$ m/d. This configuration introduces grid-orientation effects, generally resulting from approximations used to compute dispersive solute fluxes related to the cross-product terms of the dispersion tensor. This also leads to some negative concentrations at the margins of the plume. Comparison of results for applying the original and new methods to this variant of the test problem showed slightly greater differences than for the case with flow parallel to the grid. However, the most notable difference was that the new method reduced the extent of negative concentrations—a clear benefit of the new algorithm. Using the original method for adjusting particles resulted in 174 cells of the finite-difference grid having relative concentrations less than -0.01 and 339 cells with $C < -0.001$. In

contrast, at 120 days the new algorithm yielded just 16 cells with $C < -0.01$ and 29 cells with $C < -0.001$.

The use of the new algorithm only has a very small effect on computational efficiency. For the test problem with uniform flow parallel to the grid (Fig. 5), using 75 particles per cell and a Courant criterion of 0.25 required 145 time steps and about 4.7×10^6 particles; the computational time increased from 283.9 to 285.3 s for the original and new methods, respectively, a difference of about 0.5%. When the problem was modified so that flow was at a 45° angle to the grid, using 45 particles per cell and a Courant criterion of 0.25 required 121 time steps and about 3.5×10^6 particles; in this case the computational time increased from 392.1 to 393.7 s for the original and new methods, respectively, an increase of about 0.4%. For the variant of the test problem with nonuniform flow in heterogeneous media (Fig. 6), using 27 particles per cell and a Courant criterion of 0.5 required 402 time steps and about 3.5×10^6 particles; the computational time increased from 362.3 to 365.9 s for the original and new methods, respectively, a difference of almost 1 percent. These results indicate that the implementation of the new method will impose a very small additional computational burden—generally less than 1%, although the exact times and differences will be problem dependent.

6 Conclusions

The method-of-characteristics groundwater transport models, as well as some similar particle-based Eulerian–Lagrangian methods, require that changes in concentrations computed within an Eulerian framework (fixed grid) to account for dispersion be transferred to moving particles used to simulate advective transport. A new algorithm was developed to accomplish this transfer between nodal values and advecting particles more precisely and realistically, with little additional computational cost, compared to currently used methods.

The new method scales the changes and adjustments of particle concentrations relative to limiting bounds of concentration values determined from the population of adjacent nodal values, which drive the calculated dispersive fluxes into and out of the cell of interest. The method preserves realistic concentration variations within a cell and precludes unrealistic undershoot or overshoot for concentrations of individual particles. The magnitude of the concentration change will vary among particles within a cell, depending on the initial value. If dispersion is causing concentrations to decrease during a time step, those particles with the highest concentration will decrease the most, and those with the lowest concentration will decrease the least, as would be expected conceptually. The converse is true if dispersion is causing concentrations to increase. Furthermore, if the initial concentration on a particle is outside the range of the bounding cell values, it will automatically be adjusted in the direction of the acceptable range of values. The transfer process will never cause the concentration of a particle having a positive value to become negative in sign, and overall the new method will reduce the occurrence of negative concentration values calculated at nodes of grid cells. The new method also is inherently mass conservative.

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